Name: _____

PHYSICS 619 : SPRING SEMESTER 2019

Project #7: Quantum Monte Carlo Integration

1. Use the Box-Mueller method to generate a set of 3 Gaussian variables x_i, y_i, and z_i according the probability distribution

$$P(x,y,z) = \Psi_T^2(r) = N\mathrm{e}^{-2\alpha r^2},$$

where $r = \sqrt{x^2+y^2+z^2}$ and N is the normalization factor. (If you can, use BM 3 times to generate six Gaussians and use it twice). You can now compute the variational energy of hydrogen

$$\begin{aligned} E_V =< H > &= \int dxdydz\, \Psi_T H \Psi_T, \\ &= \int dxdydz\, \Psi_T^2 (\, H\, \Psi_T)/\Psi_T, \\ &= \frac{1}{n}\sum_{i=1}^{n} H\Psi_T(x_i,y_i,z_i)/\Psi_T, \end{aligned}$$

as a function of α (take α=0.05 to 0.5 in increments of 0.05 and $n = 10^5$) with

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r}.$$

Plot your variation energy as a function of α using the standard deviation error as your error bar. Hand in this plot. What is the value of α which minimizing E_V in this case? Check your numerical answer by doing the minimization analytically. What are the analytical values of α and E_V ?

2. Now use the Metropolis algorithm to sample a set of 3-D vectors $\{\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N\}$ (take $N = 10^5$) according to

$$\Psi_T^2(r) = \mathrm{e}^{-2\alpha r},$$

where $r = \sqrt{x^2+y^2+z^2}$. You do this by starting at some initial position

$$\mathbf{r} = (x,y,z),$$

change it by adding to it a random displacement vector

$$\Delta\mathbf{r} = (r_{max} * [ran(iseed) - .5], r_{max} * [ran(iseed) - .5], r_{max} * [ran(iseed) - .5]),$$

getting

$$\mathbf{r}' = \mathbf{r} + \Delta\mathbf{r},$$

and then accept or reject this new position according to the ratio

$$R = \frac{\Psi_T^2(r')}{\Psi_T^2(r)}$$

as prescribed by the Metropolis et al algorithm. Adjust r_{max} so that the proposed change is accepted about 50% to 30% of the time. After you have updated 100-200 times, (allowing the system to equilibrate to its equilibrium distribution), evaluate the variational energy

$$\begin{aligned} E_V =< H > &= \frac{\int dxdydz\, \Psi_T H \Psi_T}{\int dxdydz\, \Psi_T^2}, \\ &= \frac{\int dxdydz\, \Psi_T^2 (\Psi^{-1}\, H\, \Psi_T)}{\int dxdydz\, \Psi_T^2}, \\ &= \frac{1}{n}\sum_{i=1}^{n} \Psi^{-1} H \Psi_T(\mathbf{r}_i), \end{aligned}$$

as a function of α (take α=0.2 to 2.0 in increments of 0.2) with

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r}.$$

Plot your variation energy as a function of α and use the standard error as your error bar. Hand in this plot. (Don't forget to divide by $1/\sqrt{n}$ where n is the number of configurations you averaged over. Ideally n should be number of independent configurations. If your error bars are very small, you have *over estimated* your number of independent configurations.) Plot in the same graph, also a curve corresponding to the expected theoretical result

$$E_V = \frac{1}{2}\alpha^2 - \alpha.$$

Comment on the comparison.

3. Now, do the calculation for the Helium atom case with (in atomic units)

$$\Psi_T^2(r_1, r_2) = \mathrm{e}^{-2\alpha r_1}\mathrm{e}^{-2\alpha r_2}.$$

and

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}.$$

What is the minimizing value for α in this case? (Check your numerical answer by doing the minimization analytically.) What is the corresponding minimum value for E_V?